



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:28 PM UTC

PDB ID : 2EAV / pdb\_00002eav  
Title : Crystal structure of the C-terminal peptidoglycan-binding domain of human peptidoglycan recognition protein Ibeta  
Authors : Cho, S.; Mariuzza, R.A.  
Deposited on : 2007-02-03  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

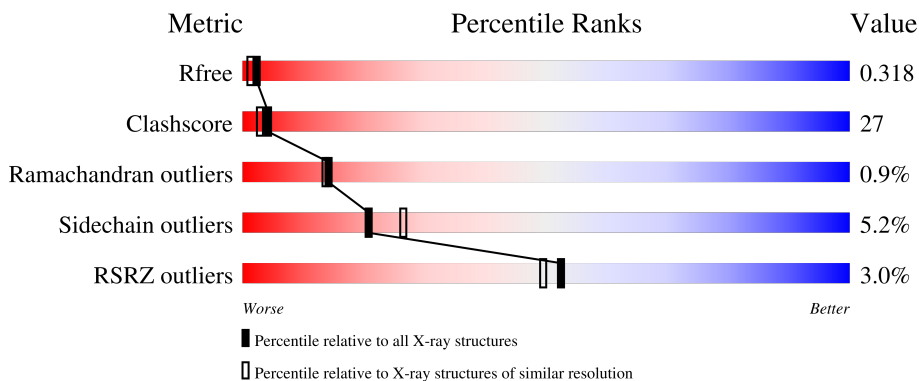
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	165	 2% 52% 44% ..
1	B	165	 4% 58% 37% ..

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2663 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Peptidoglycan recognition protein-I-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	164	1259	802	217	231	9	0	0	0
1	B	164	1259	802	217	231	9	0	0	0

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Ni 2	0	0
2	B	4	Total 4	Ni 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	73	Total 73	O 73	0	0
3	B	66	Total 66	O 66	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.44Å 56.78Å 36.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 30.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.7 (30.00-2.20) 91.6 (30.00-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 1.95Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.229 , 0.285 0.232 , 0.318	Depositor DCC
$R_{free}$ test set	785 reflections (5.27%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.4	Xtrriage
Anisotropy	0.465	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 51.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2663	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NI

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.43	0/1292	1.01	7/1760 (0.4%)
1	B	0.45	0/1292	0.98	5/1760 (0.3%)
All	All	0.44	0/2584	1.00	12/3520 (0.3%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	ASP	N-CA-C	-7.16	104.58	113.38
1	B	222	ARG	CB-CA-C	6.91	121.20	109.53
1	B	236	GLY	N-CA-C	-6.36	98.11	113.18
1	A	265	ASP	N-CA-C	6.34	119.42	111.24
1	B	309	PHE	N-CA-C	-6.00	100.79	110.32
1	B	281	ASP	N-CA-C	-5.96	106.09	113.19
1	B	291	ASN	N-CA-C	5.94	120.53	113.16
1	A	294	GLY	N-CA-C	-5.53	104.14	112.60
1	A	339	LEU	N-CA-C	-5.52	101.18	109.95
1	A	328	ASP	N-CA-C	-5.27	105.54	111.28
1	A	211	PRO	N-CA-C	5.05	118.30	111.22
1	A	291	ASN	N-CA-C	5.03	119.41	113.28

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1259	0	1229	71	0
1	B	1259	0	1229	70	1
2	A	2	0	0	0	0
2	B	4	0	0	0	0
3	A	73	0	0	1	0
3	B	66	0	0	1	0
All	All	2663	0	2458	136	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (136) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ILE:HB	1:A:308:THR:HB	1.53	0.91
1:B:357:PRO:HB2	1:B:361:LEU:HD13	1.55	0.89
1:B:248:ILE:HD13	1:B:248:ILE:H	1.45	0.82
1:B:245:THR:HG22	1:B:311:GLY:HA3	1.63	0.79
1:A:255:LEU:O	1:A:259:ILE:HG13	1.86	0.74
1:B:344:LEU:HD22	1:B:372:LYS:HD3	1.71	0.73
1:A:357:PRO:HG2	1:A:361:LEU:HD22	1.71	0.72
1:B:247:ASN:HD22	1:B:280:GLN:HB2	1.56	0.70
1:A:228:ARG:NH1	1:A:291:ASN:HB3	2.09	0.67
1:B:239:ILE:HG12	1:B:348:HIS:HB2	1.76	0.67
1:A:264:ILE:HD11	1:A:271:ASP:HA	1.77	0.65
1:B:371:PHE:CE2	1:B:373:HIS:HB3	2.32	0.65
1:A:334:MET:HE3	1:B:331:GLN:NE2	2.11	0.64
1:B:248:ILE:HD13	1:B:248:ILE:N	2.12	0.64
1:B:266:ARG:HA	1:B:266:ARG:HE	1.62	0.63
1:A:228:ARG:HH12	1:A:291:ASN:HB3	1.64	0.63
1:A:334:MET:HG3	1:A:335:VAL:N	2.14	0.63
1:A:295:SER:HA	1:A:301:ASP:OD1	1.98	0.62
1:B:247:ASN:HD21	1:B:280:GLN:HE21	1.48	0.61
1:B:240:HIS:NE2	1:B:356:SER:HA	2.16	0.61
1:A:255:LEU:HD22	1:A:259:ILE:HD11	1.83	0.60
1:B:222:ARG:HG2	1:B:260:GLN:OE1	2.00	0.60
1:B:239:ILE:HG22	1:B:240:HIS:N	2.16	0.59
1:A:235:TYR:HB2	1:A:304:ALA:HB2	1.83	0.59
1:B:272:ILE:HD13	1:B:273:GLY:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:LEU:O	1:A:255:LEU:HD23	2.02	0.59
1:A:231:LEU:HB3	1:A:232:PRO:HA	1.84	0.58
1:A:320:ALA:O	1:A:324:GLU:HG3	2.03	0.58
1:B:214:VAL:HG13	1:B:284:ILE:O	2.04	0.58
1:A:216:ARG:HB3	1:A:221:ALA:HB3	1.85	0.58
1:A:232:PRO:HB3	1:A:337:GLY:O	2.04	0.58
1:A:307:ILE:HD12	1:A:330:ILE:CD1	2.34	0.58
1:A:238:ILE:HG21	1:A:361:LEU:HD21	1.86	0.57
1:B:288:VAL:HB	1:B:292:VAL:HB	1.87	0.57
1:A:248:ILE:HG13	1:A:251:GLU:HB3	1.85	0.57
1:A:361:LEU:C	1:A:361:LEU:HD23	2.31	0.56
1:A:357:PRO:CG	1:A:361:LEU:HD22	2.35	0.56
1:A:326:ALA:O	1:A:330:ILE:HG12	2.06	0.56
1:A:274:TYR:CG	1:A:308:THR:HG21	2.41	0.56
1:A:247:ASN:HD22	1:A:247:ASN:H	1.53	0.55
1:B:271:ASP:OD1	1:B:272:ILE:N	2.36	0.55
1:A:307:ILE:HD12	1:A:330:ILE:HD11	1.88	0.55
1:A:327:GLN:HB2	1:B:369:PRO:HG3	1.88	0.55
1:A:324:GLU:OE1	1:B:371:PHE:HB3	2.07	0.55
1:B:240:HIS:O	1:B:240:HIS:CD2	2.60	0.54
1:B:277:LEU:HD12	1:B:277:LEU:N	2.23	0.54
1:B:366:SER:HA	1:B:371:PHE:CG	2.42	0.54
1:B:229:MET:HE1	1:B:305:LEU:CD2	2.38	0.54
1:B:232:PRO:HG2	1:B:340:THR:HG22	1.89	0.54
1:A:278:VAL:HG22	1:A:284:ILE:HD12	1.89	0.54
1:B:219:TRP:CH2	1:B:221:ALA:HB2	2.43	0.54
1:A:255:LEU:CD2	1:A:259:ILE:HD11	2.37	0.53
1:B:357:PRO:HB2	1:B:361:LEU:CD1	2.34	0.53
1:A:357:PRO:HB2	1:A:361:LEU:HD13	1.91	0.52
1:B:215:PRO:HG2	1:B:218:VAL:HG23	1.92	0.52
1:B:373:HIS:CD2	1:B:373:HIS:H	2.26	0.52
1:B:349:SER:HB3	1:B:356:SER:O	2.10	0.52
1:B:355:LEU:H	1:B:355:LEU:HD22	1.76	0.51
1:B:239:ILE:O	1:B:308:THR:HA	2.10	0.51
1:B:241:THR:HG23	1:B:310:MET:HA	1.92	0.51
1:B:255:LEU:HD13	1:B:310:MET:SD	2.50	0.51
1:B:276:PHE:C	1:B:277:LEU:HD12	2.35	0.51
1:A:343:TYR:O	1:A:370:HIS:HB3	2.12	0.50
1:A:346:VAL:HG12	1:A:372:LYS:HB3	1.92	0.50
1:A:226:CYS:HB3	1:A:227:PRO:HD2	1.92	0.50
1:B:366:SER:HA	1:B:371:PHE:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:PRO:HG2	1:A:218:VAL:HG23	1.94	0.50
1:B:239:ILE:CG2	1:B:240:HIS:N	2.75	0.50
1:B:371:PHE:HE2	1:B:373:HIS:HB3	1.75	0.50
1:B:261:SER:HB3	1:B:265:ASP:OD1	2.13	0.49
1:B:355:LEU:H	1:B:355:LEU:CD2	2.25	0.49
1:B:250:ASP:OD2	1:B:251:GLU:N	2.45	0.49
1:B:371:PHE:CD2	1:B:373:HIS:HB3	2.46	0.49
1:A:264:ILE:O	1:A:268:LYS:HA	2.12	0.49
1:A:360:ALA:O	1:A:364:ILE:HD13	2.12	0.49
1:B:344:LEU:CD2	1:B:372:LYS:HD3	2.41	0.48
1:B:250:ASP:OD2	1:B:250:ASP:C	2.57	0.48
1:B:253:ARG:HH21	1:B:253:ARG:HG3	1.78	0.48
1:A:248:ILE:HD11	3:A:105:HOH:O	2.14	0.48
1:A:361:LEU:HD23	1:A:361:LEU:O	2.14	0.48
1:A:369:PRO:HG3	1:B:327:GLN:HB2	1.96	0.48
1:A:226:CYS:HB3	1:A:227:PRO:CD	2.44	0.47
1:A:275:ASN:HA	1:A:288:VAL:HG22	1.96	0.47
1:B:261:SER:O	1:B:265:ASP:HB2	2.15	0.47
1:A:355:LEU:HD13	1:A:355:LEU:O	2.15	0.46
1:B:344:LEU:HD22	1:B:372:LYS:HB2	1.98	0.46
1:A:240:HIS:CD2	1:A:240:HIS:O	2.67	0.46
1:A:274:TYR:CD1	1:A:308:THR:HG21	2.51	0.46
1:B:373:HIS:CD2	1:B:373:HIS:N	2.83	0.46
1:B:355:LEU:O	1:B:356:SER:C	2.58	0.46
1:A:277:LEU:HA	1:A:308:THR:O	2.15	0.46
1:A:284:ILE:HD11	1:A:325:ALA:HB1	1.97	0.46
1:A:239:ILE:HG23	1:A:348:HIS:ND1	2.31	0.46
1:A:334:MET:HE3	1:B:331:GLN:CD	2.40	0.46
1:A:353:ARG:HD3	1:A:353:ARG:C	2.41	0.46
1:A:247:ASN:HD22	1:A:247:ASN:N	2.09	0.46
1:B:355:LEU:HD22	1:B:355:LEU:N	2.30	0.45
1:A:239:ILE:HG22	1:A:240:HIS:N	2.32	0.45
1:B:334:MET:HE3	1:B:334:MET:HA	1.96	0.45
1:B:346:VAL:HG12	1:B:372:LYS:HB3	1.97	0.45
1:A:315:GLY:C	1:A:316:ILE:HG13	2.41	0.45
1:A:244:ARG:NH1	1:A:258:ASP:OD2	2.44	0.45
1:A:364:ILE:HD12	1:A:364:ILE:N	2.31	0.45
1:B:280:GLN:C	1:B:282:GLY:H	2.24	0.45
1:A:216:ARG:HB3	1:A:221:ALA:CB	2.45	0.44
1:A:276:PHE:HD2	1:A:286:GLU:HA	1.82	0.44
1:A:248:ILE:HG13	1:A:251:GLU:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:LYS:O	1:B:372:LYS:HG3	2.18	0.44
1:A:250:ASP:OD2	1:A:253:ARG:NH1	2.51	0.44
1:B:275:ASN:OD1	1:B:305:LEU:HA	2.18	0.44
1:B:360:ALA:O	1:B:364:ILE:HG12	2.18	0.43
1:A:276:PHE:CD2	1:A:286:GLU:HA	2.54	0.43
1:B:210:CYS:N	3:B:114:HOH:O	2.51	0.43
1:A:336:LYS:HE2	1:A:336:LYS:HB3	1.85	0.43
1:A:235:TYR:HB2	1:A:304:ALA:CB	2.47	0.42
1:B:248:ILE:N	1:B:248:ILE:CD1	2.82	0.42
1:A:241:THR:O	1:A:242:ALA:HB3	2.18	0.42
1:B:222:ARG:HG2	1:B:222:ARG:H	1.66	0.42
1:B:261:SER:O	1:B:265:ASP:N	2.47	0.42
1:B:280:GLN:C	1:B:282:GLY:N	2.77	0.42
1:B:280:GLN:HB3	1:B:319:ASN:ND2	2.34	0.42
1:B:316:ILE:HD12	1:B:317:PRO:HD2	2.01	0.42
1:A:240:HIS:O	1:A:240:HIS:HD2	2.02	0.42
1:B:317:PRO:HD3	1:B:360:ALA:HB1	2.02	0.42
1:A:307:ILE:HD13	1:A:329:LEU:HD23	2.02	0.42
1:A:246:CYS:HB2	1:A:251:GLU:HG2	2.02	0.41
1:B:216:ARG:HB3	1:B:221:ALA:HB3	2.02	0.41
1:A:247:ASN:N	1:A:247:ASN:ND2	2.67	0.41
1:A:240:HIS:CD2	1:A:357:PRO:HA	2.55	0.41
1:A:219:TRP:CH2	1:A:221:ALA:HB2	2.56	0.41
1:A:239:ILE:O	1:A:308:THR:HA	2.20	0.41
1:A:355:LEU:HA	1:A:355:LEU:HD22	1.86	0.41
1:B:234:LYS:HG2	1:B:303:ILE:HB	2.03	0.40
1:B:240:HIS:CD2	1:B:357:PRO:HA	2.55	0.40
1:A:279:GLY:C	1:A:281:ASP:H	2.28	0.40
1:B:280:GLN:HB3	1:B:319:ASN:HD21	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:HIS:OXT	1:B:373:HIS:OXT[2_555]	1.98	0.22

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	162/165 (98%)	149 (92%)	11 (7%)	2 (1%)	10	8
1	B	162/165 (98%)	150 (93%)	11 (7%)	1 (1%)	21	23
All	All	324/330 (98%)	299 (92%)	22 (7%)	3 (1%)	14	14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	HIS
1	A	249	SER
1	B	353	ARG

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	134/134 (100%)	127 (95%)	7 (5%)	21	26
1	B	134/134 (100%)	127 (95%)	7 (5%)	21	26
All	All	268/268 (100%)	254 (95%)	14 (5%)	21	26

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	VAL
1	A	231	LEU
1	A	234	LYS

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Mol	Chain	Res	Type
1	A	247	ASN
1	A	334	MET
1	A	336	LYS
1	A	355	LEU
1	B	214	VAL
1	B	222	ARG
1	B	248	ILE
1	B	255	LEU
1	B	272	ILE
1	B	361	LEU
1	B	373	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	HIS
1	A	247	ASN
1	A	327	GLN
1	A	331	GLN
1	B	247	ASN
1	B	293	GLN
1	B	327	GLN
1	B	373	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	164/165 (99%)	0.12	3 (1%) 67 64	17, 26, 38, 51	0
1	B	164/165 (99%)	0.24	7 (4%) 40 36	16, 26, 44, 67	0
All	All	328/330 (99%)	0.18	10 (3%) 52 49	16, 26, 41, 67	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	356	SER	5.3
1	B	373	HIS	4.8
1	B	357	PRO	3.9
1	A	210	CYS	2.9
1	A	353	ARG	2.9
1	B	355	LEU	2.8
1	B	353	ARG	2.7
1	B	354	THR	2.1
1	A	324	GLU	2.0
1	B	372	LYS	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NI	A	504	1/1	0.92	0.17	61,61,61,61	0
2	NI	A	501	1/1	0.96	0.16	35,35,35,35	0
2	NI	B	500	1/1	0.97	0.10	30,30,30,30	0
2	NI	B	502	1/1	0.97	0.08	39,39,39,39	0
2	NI	B	505	1/1	0.97	0.06	47,47,47,47	0
2	NI	B	503	1/1	0.98	0.14	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.